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Crystal structure of *N*,*N*-dimethyl-2-[(4-methylbenzyl)sulfonyl]ethanamine

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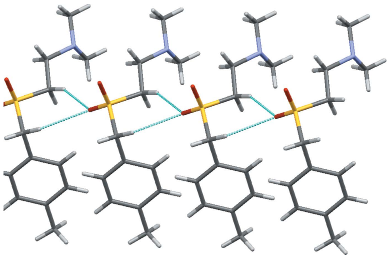
In the crystal, the title compound, $C_{12}H_{19}NO_2S$, has a disordered structure with two equally populated conformations of the amine fragment. A pair of weak $C-H\cdots O$ intermolecular interactions between the CH_2 and SO_2 groups gives a one-dimensional supramolecular structure that propagates through translation along the *a*-axis direction.



1. Chemical context

Parasitic helminths possess a number of evolutionary strategies that facilitate their co-existence with their host and, as such, up to one third of the global population may suffer from helminthetic infections (de Silva *et al.*, 2003). These parasites can secrete immunomodulatory molecules that prevent the parasites' clearance from the host without leaving the host vulnerable to opportunistic infections (Hewitson *et al.*, 2009). ES-62 is one such immunomodulatory molecule, a protein, which was discovered in the secretions of the rodent filarial nematode *Acanthocheilonema* and demonstrated to induce an anti-inflammatory immunological phenotype (Harnett *et al.*, 1989). ES-62 has been studied for its potential to treat human diseases relating to inflammation, for example collagen-induced arthritis or rheumatoid arthritis, and many positive outcomes have been demonstrated.

A number of the significant anti-inflammatory activities of ES-62 are associated with post-translational glycosylation and subsequent esterification by phosphorylcholine. However, ES-62 is an immunogenic protein and is thus unsuitable as a drug itself (Harnett & Harnett, 2009). We have sought to capitalize on the immunomodulatory effects of ES-62 whilst avoiding its inherent undrugability through synthesizing a library of drug-like small molecules based upon phosphorylcholine, the active moiety of ES-62. A series of sulfone analogues (Fig. 1) have proven to be of great significance in our investigations into

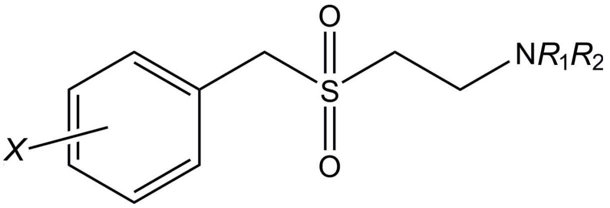
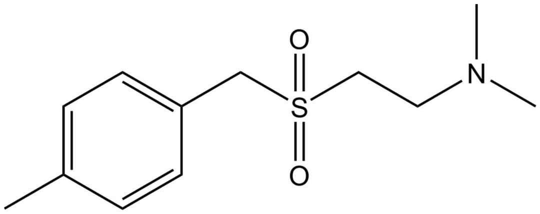


Figure 1
General structure of sulfone analogues. *R* represents alkyl chains and *X* represents halogen substituents.

collagen-induced arthritis. Despite the apparent simplicity of these molecules, we are aware of no relevant crystallographic study. As such, and as the title compound is of particular interest to our ongoing work (Al-Riyami *et al.*, 2013), we report herein on the solid-state structure of the title compound.



2. Structural commentary

The molecular structure of the title compound is shown in Fig. 2. The amine group is disordered over two equally occupied sites such that the lone pair of the pyramidal N atom is *anti* to O1 with respect to the plane defined by C1—S1—C9 for the conformer containing N1 but *syn* for the N1*A* conformer.

3. Supramolecular features

Neighbouring molecules related by translation along the *a*-axis direction are connected by two weak C—H⋯O hydrogen bonds involving O1 and C1 and C9/C9*A* (Table 1 and Fig. 3). This gives one-dimensional supramolecular chains of molecules that propagate parallel to the crystallographic *a*-axis direction.

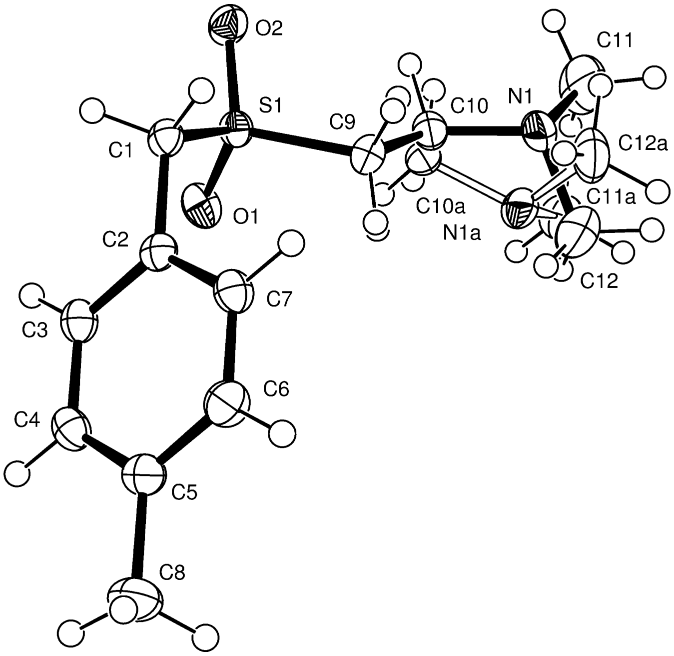


Figure 2
The molecular structure of the title compound with non-H atoms shown as 50% probability displacement ellipsoids. For the disordered fragment, the atoms labelled with the suffix 'a' have been shown with hollow bonds whilst all other bonds are shown as solid lines.

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C1—H1*A*⋯O1^{i}	0.99	2.60	3.493 (2)	150
C9—H9*A*⋯O1^{i}	0.99	2.49	3.415 (2)	155
C9*A*—H9*C*⋯O1^{i}	0.99	2.61	3.415 (2)	138

Symmetry code: (i) $x - 1, y, z$.

Other close interactions involve the disordered fragment. Thus the methyl group of C11*A* approaches the aromatic ring, giving a C—ċπ interaction [closest contact C6⋯C11*A* = 3.345 (5) Å] whilst C11 forms unfeasibly short intermolecular interactions with its centrosymmetrically related self – an interaction that is relieved by the observed disorder.

4. Synthesis and crystallization

A mixture of 2-[(4-methylbenzyl)sulfonyl]ethyl methanesulfonate and 1-methyl-4-[(vinylsulfonyl)methyl]benzene (4.880 g) was dissolved in dichloromethane (50 ml, dry) to which dimethylamine (4 ml, 2*M* in THF) was added at room temperature with stirring. The stirring was continued at room temperature overnight. The reaction mixture was extracted with a saturated solution of sodium carbonate. The organic layer was collected, dried over $MgSO_4$, filtered and the solvents were removed under reduced pressure and the crude product was applied to a silica gel column chromatography using first ethyl acetate/*n*-hexane (1/1, RF = 0.1) and then ethyl acetate/methanol (9/1). The product was obtained as a white solid which was recrystallized from ethyl acetate/*n*-hexane (2.200 g) (m.p. 341–343 K). HRESIMS: calculated for $C_{12}H_{19}NO_2S$, 241.1136; found: 241.1139.

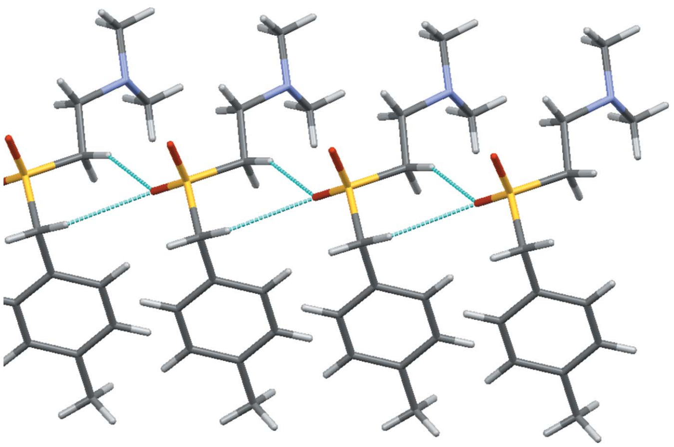


Figure 3
Part of the molecular chain formed by translation along *a* highlighting the C—H⋯O contacts. Only one of the two disordered conformations is shown.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Models where the site occupancy factors of the disordered groups were allowed to refine gave occupancies equal to 50%. So in the final model, occupancies of all the disordered atoms were set to this value. The C9—C10 and C9*A*—C10*A* distances were restrained to be 1.53 (1) Å. All H atoms were placed in idealized positions and were refined in riding modes with C—H equal to 0.95, 0.98 and 0.99 Å for CH, CH_2 and CH_3 groups, respectively, and U_{iso}(H) = $1.5U_{eq}$(C) for methyl groups and $1.2U_{eq}$(C) for all other groups.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{19}NO_2S$
M_r	241.34
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	123
a, *b*, *c* (Å)	5.3642 (3), 10.3773 (6), 12.1784 (7)
α, β, γ (°)	99.572 (5), 95.498 (5), 104.645 (5)
V (Å^3)	639.98 (6)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	2.14
Crystal size (mm)	0.30 × 0.10 × 0.03
Data collection	
Diffractometer	Oxford Diffraction Gemini S
Absorption correction	Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min}, T_{max}	0.459, 0.938
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5846, 2491, 2360
R_{int}	0.023
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.620
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.121, 1.08
No. of reflections	2491
No. of parameters	186
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.48, −0.36

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2009), *SIR92* (Altomare *et al.*, 1994), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

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supporting information

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Crystal structure of *N*,*N*-dimethyl-2-[(4-methylbenzyl)sulfonyl]ethanamine

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2009); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2009); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

N,*N*-Dimethyl-2-[(4-methylbenzyl)sulfonyl]ethanamine

Crystal data

$C_{12}H_{19}NO_2S$
$M_r = 241.34$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.3642\ (3)$ Å
$b = 10.3773\ (6)$ Å
$c = 12.1784\ (7)$ Å
$\alpha = 99.572\ (5)°$
$\beta = 95.498\ (5)°$
$\gamma = 104.645\ (5)°$
$V = 639.98\ (6)$ Å^3

$Z = 2$
$F(000) = 260$
$D_x = 1.252$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 3570 reflections
$\theta = 5.2–72.9°$
$\mu = 2.14$ mm^{-1}
$T = 123$ K
Plate, colourless
0.30 × 0.10 × 0.03 mm

Data collection

Oxford Diffraction Gemini S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min} = 0.459$, $T_{max} = 0.938$

5846 measured reflections
2491 independent reflections
2360 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 72.9°$, $\theta_{min} = 3.7°$
$h = -4 \rightarrow 6$
$k = -12 \rightarrow 11$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.121$
$S = 1.08$
2491 reflections
186 parameters
2 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.2621P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

Experimental. ^{1}H NMR (DMSO-d$_6$): δ 7.28 (2*H*, d, J = 8.0 Hz), 7.21 (2*H*, d, J = 8.0 Hz), 4.44 (2*H*, s), 3.17 (2*H*, t, J = 14.3 Hz), 2.65 (2*H*, t, J = 14.3 Hz), 2.31 (3*H*, s), 2.16 (6*H*, s). ^{13}C NMR (DMSO-d$_6$): δ 137.7, 130.8, 129.0, 125.4, 58.4, 51.6, 49.0, 44.9, 20.7. IR (KBr): 1511, 1463, 1399, 1380, 1314, 1258, 1156, 1119, 1050, 892, 853, 822, 749 cm^{-1}.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.89090 (7)	0.52015 (4)	0.66118 (3)	0.02154 (16)	
O1	1.1289 (2)	0.48170 (12)	0.68167 (11)	0.0307 (3)	
O2	0.9042 (2)	0.63679 (12)	0.60940 (10)	0.0295 (3)	
C1	0.6462 (3)	0.38079 (16)	0.57471 (13)	0.0223 (3)	
H1A	0.4763	0.4021	0.5740	0.027*	
H1B	0.6866	0.3706	0.4966	0.027*	
C2	0.6217 (3)	0.24813 (16)	0.61229 (13)	0.0211 (3)	
C3	0.7832 (3)	0.16706 (17)	0.57982 (14)	0.0252 (4)	
H3	0.9114	0.1961	0.5338	0.030*	
C4	0.7579 (3)	0.04422 (17)	0.61421 (14)	0.0259 (4)	
H4	0.8692	−0.0101	0.5912	0.031*	
C5	0.5729 (3)	−0.00109 (17)	0.68174 (14)	0.0262 (4)	
C6	0.4119 (4)	0.08042 (18)	0.71320 (16)	0.0300 (4)	
H6	0.2838	0.0513	0.7592	0.036*	
C7	0.4342 (3)	0.20319 (17)	0.67902 (14)	0.0253 (4)	
H7	0.3211	0.2568	0.7012	0.030*	
C8	0.5437 (4)	−0.13542 (19)	0.71811 (18)	0.0377 (5)	
H8A	0.5787	−0.1201	0.8004	0.057*	
H8B	0.6676	−0.1802	0.6856	0.057*	
H8C	0.3659	−0.1933	0.6920	0.057*	
C9	0.7696 (3)	0.55043 (17)	0.79112 (14)	0.0248 (4)	0.50
H9A	0.5883	0.5562	0.7768	0.030*	0.50
H9B	0.7692	0.4741	0.8304	0.030*	0.50
N1	0.8311 (7)	0.7301 (3)	0.9652 (3)	0.0333 (7)	0.50
C10	0.9410 (19)	0.6837 (8)	0.8655 (9)	0.0264 (18)	0.50
H10A	1.1132	0.6711	0.8900	0.032*	0.50
H10B	0.9689	0.7554	0.8200	0.032*	0.50
C11	0.9697 (14)	0.8715 (5)	1.0135 (4)	0.0648 (15)	0.50
H11A	0.8822	0.9060	1.0743	0.097*	0.50

H11B	0.9707	0.9261	0.9551	0.097*	0.50
H11C	1.1492	0.8774	1.0435	0.097*	0.50
C12	0.8399 (16)	0.6456 (6)	1.0475 (5)	0.0683 (18)	0.50
H12A	0.7464	0.5512	1.0134	0.102*	0.50
H12B	0.7577	0.6770	1.1114	0.102*	0.50
H12C	1.0216	0.6513	1.0737	0.102*	0.50
N1A	0.9175 (6)	0.6553 (3)	0.9889 (3)	0.0297 (7)	0.50
C9A	0.7696 (3)	0.55043 (17)	0.79112 (14)	0.0248 (4)	0.50
H9C	0.6106	0.5813	0.7797	0.030*	0.50
H9D	0.7240	0.4654	0.8207	0.030*	0.50
C10A	0.9780 (18)	0.6589 (8)	0.8749 (8)	0.0231 (17)	0.50
H10C	1.1504	0.6423	0.8688	0.028*	0.50
H10D	0.9848	0.7496	0.8578	0.028*	0.50
C11A	1.1294 (9)	0.7511 (4)	1.0688 (3)	0.0394 (9)	0.50
H11D	1.2931	0.7284	1.0582	0.059*	0.50
H11E	1.0940	0.7461	1.1457	0.059*	0.50
H11F	1.1434	0.8434	1.0563	0.059*	0.50
C12A	0.6727 (9)	0.6851 (5)	1.0055 (4)	0.0424 (10)	0.50
H12D	0.6451	0.6851	1.0839	0.064*	0.50
H12E	0.5301	0.6158	0.9554	0.064*	0.50
H12F	0.6772	0.7746	0.9884	0.064*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0207 (2)	0.0219 (2)	0.0214 (2)	0.00508 (16)	0.00401 (15)	0.00319 (16)
O1	0.0228 (6)	0.0307 (7)	0.0357 (7)	0.0074 (5)	0.0033 (5)	−0.0006 (5)
O2	0.0357 (7)	0.0258 (6)	0.0264 (6)	0.0050 (5)	0.0073 (5)	0.0071 (5)
C1	0.0221 (8)	0.0237 (8)	0.0190 (7)	0.0053 (6)	0.0001 (6)	0.0018 (6)
C2	0.0199 (7)	0.0219 (8)	0.0182 (7)	0.0031 (6)	−0.0027 (6)	0.0016 (6)
C3	0.0220 (8)	0.0285 (9)	0.0240 (8)	0.0066 (7)	0.0043 (6)	0.0018 (7)
C4	0.0231 (8)	0.0255 (8)	0.0267 (8)	0.0084 (6)	−0.0005 (6)	−0.0011 (7)
C5	0.0261 (8)	0.0231 (8)	0.0258 (8)	0.0039 (6)	−0.0023 (6)	0.0031 (6)
C6	0.0275 (9)	0.0309 (9)	0.0327 (9)	0.0060 (7)	0.0102 (7)	0.0094 (7)
C7	0.0218 (8)	0.0274 (8)	0.0265 (8)	0.0079 (7)	0.0041 (6)	0.0029 (7)
C8	0.0437 (11)	0.0273 (9)	0.0433 (11)	0.0098 (8)	0.0056 (9)	0.0110 (8)
C9	0.0252 (8)	0.0284 (8)	0.0200 (8)	0.0062 (7)	0.0042 (6)	0.0043 (6)
N1	0.045 (2)	0.0337 (17)	0.0244 (16)	0.0202 (16)	0.0042 (15)	0.0002 (13)
C10	0.024 (3)	0.034 (3)	0.022 (3)	0.013 (2)	−0.0005 (19)	0.001 (2)
C11	0.106 (5)	0.042 (3)	0.037 (2)	0.017 (3)	0.006 (3)	−0.011 (2)
C12	0.121 (6)	0.066 (4)	0.033 (3)	0.045 (4)	0.025 (3)	0.016 (3)
N1A	0.0366 (17)	0.0302 (17)	0.0197 (17)	0.0083 (14)	−0.0003 (13)	0.0013 (13)
C9A	0.0252 (8)	0.0284 (8)	0.0200 (8)	0.0062 (7)	0.0042 (6)	0.0043 (6)
C10A	0.023 (3)	0.027 (3)	0.019 (2)	0.009 (2)	−0.0031 (18)	0.003 (2)
C11A	0.046 (2)	0.040 (2)	0.0253 (18)	0.0098 (18)	−0.0103 (16)	−0.0028 (16)
C12A	0.046 (2)	0.053 (3)	0.028 (2)	0.020 (2)	0.0083 (19)	−0.0024 (18)

Geometric parameters (Å, º)

S1—O1	1.4426 (13)	C9—H9B	0.9900
S1—O2	1.4446 (12)	N1—C12	1.442 (6)
S1—C9	1.7780 (16)	N1—C11	1.460 (6)
S1—C1	1.7867 (16)	N1—C10	1.462 (12)
C1—C2	1.501 (2)	C10—H10A	0.9900
C1—H1A	0.9900	C10—H10B	0.9900
C1—H1B	0.9900	C11—H11A	0.9800
C2—C7	1.391 (2)	C11—H11B	0.9800
C2—C3	1.392 (2)	C11—H11C	0.9800
C3—C4	1.386 (2)	C12—H12A	0.9800
C3—H3	0.9500	C12—H12B	0.9800
C4—C5	1.390 (3)	C12—H12C	0.9800
C4—H4	0.9500	N1A—C12A	1.448 (6)
C5—C6	1.390 (2)	N1A—C11A	1.457 (5)
C5—C8	1.507 (2)	N1A—C10A	1.460 (12)
C6—C7	1.385 (2)	C10A—H10C	0.9900
C6—H6	0.9500	C10A—H10D	0.9900
C7—H7	0.9500	C11A—H11D	0.9800
C8—H8A	0.9800	C11A—H11E	0.9800
C8—H8B	0.9800	C11A—H11F	0.9800
C8—H8C	0.9800	C12A—H12D	0.9800
C9—C10	1.536 (7)	C12A—H12E	0.9800
C9—H9A	0.9900	C12A—H12F	0.9800
O1—S1—O2	117.10 (8)	H8B—C8—H8C	109.5
O1—S1—C9	108.51 (8)	C10—C9—S1	109.9 (5)
O2—S1—C9	108.29 (8)	C10—C9—H9A	109.7
O1—S1—C1	109.89 (7)	S1—C9—H9A	109.7
O2—S1—C1	107.22 (7)	C10—C9—H9B	109.7
C9—S1—C1	105.17 (8)	S1—C9—H9B	109.7
C2—C1—S1	113.98 (11)	H9A—C9—H9B	108.2
C2—C1—H1A	108.8	C12—N1—C11	110.8 (4)
S1—C1—H1A	108.8	C12—N1—C10	111.7 (5)
C2—C1—H1B	108.8	C11—N1—C10	109.5 (5)
S1—C1—H1B	108.8	N1—C10—C9	113.9 (8)
H1A—C1—H1B	107.7	N1—C10—H10A	108.8
C7—C2—C3	118.87 (15)	C9—C10—H10A	108.8
C7—C2—C1	120.38 (14)	N1—C10—H10B	108.8
C3—C2—C1	120.74 (14)	C9—C10—H10B	108.8
C4—C3—C2	120.35 (15)	H10A—C10—H10B	107.7
C4—C3—H3	119.8	C12A—N1A—C11A	110.2 (3)
C2—C3—H3	119.8	C12A—N1A—C10A	112.8 (4)
C3—C4—C5	121.28 (15)	C11A—N1A—C10A	109.0 (4)
C3—C4—H4	119.4	N1A—C10A—H10C	109.8
C5—C4—H4	119.4	N1A—C10A—H10D	109.8
C4—C5—C6	117.86 (16)	H10C—C10A—H10D	108.2

C4—C5—C8	121.24 (16)	N1A—C11A—H11D	109.5
C6—C5—C8	120.90 (16)	N1A—C11A—H11E	109.5
C7—C6—C5	121.50 (16)	H11D—C11A—H11E	109.5
C7—C6—H6	119.3	N1A—C11A—H11F	109.5
C5—C6—H6	119.3	H11D—C11A—H11F	109.5
C6—C7—C2	120.15 (15)	H11E—C11A—H11F	109.5
C6—C7—H7	119.9	N1A—C12A—H12D	109.5
C2—C7—H7	119.9	N1A—C12A—H12E	109.5
C5—C8—H8A	109.5	H12D—C12A—H12E	109.5
C5—C8—H8B	109.5	N1A—C12A—H12F	109.5
H8A—C8—H8B	109.5	H12D—C12A—H12F	109.5
C5—C8—H8C	109.5	H12E—C12A—H12F	109.5
H8A—C8—H8C	109.5		

O1—S1—C1—C2	47.30 (14)	C8—C5—C6—C7	−179.06 (16)
O2—S1—C1—C2	175.57 (11)	C5—C6—C7—C2	−0.4 (3)
C9—S1—C1—C2	−69.31 (13)	C3—C2—C7—C6	0.7 (2)
S1—C1—C2—C7	96.45 (16)	C1—C2—C7—C6	179.81 (14)
S1—C1—C2—C3	−84.47 (17)	O1—S1—C9—C10	72.2 (3)
C7—C2—C3—C4	−0.4 (2)	O2—S1—C9—C10	−55.9 (3)
C1—C2—C3—C4	−179.51 (14)	C1—S1—C9—C10	−170.2 (3)
C2—C3—C4—C5	−0.2 (3)	C12—N1—C10—C9	71.5 (7)
C3—C4—C5—C6	0.5 (3)	C11—N1—C10—C9	−165.3 (5)
C3—C4—C5—C8	179.36 (16)	S1—C9—C10—N1	169.5 (4)
C4—C5—C6—C7	−0.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O1$^{\text{i}}$	0.99	2.60	3.493 (2)	150
C9—H9*A*···O1$^{\text{i}}$	0.99	2.49	3.415 (2)	155
C9*A*—H9*C*···O1$^{\text{i}}$	0.99	2.61	3.415 (2)	138

Symmetry code: (i) $x-1, y, z$.